Abstract No. Huck594

Buckling of the CuO_2 planes in a $La_{2-x}Ba_xCuO_4$ film (x=1/8) on a $SrTiO_3$ substrate

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Beamline(s): X22C

Introduction: In bulk samples of the famous high temperature superconductor $La_{2-x}Ba_xCuO_4$ (LBCO) a very interesting interplay between structural and electronic degrees of freedom has been observed. In this compound superconductivity is suppressed at x=1/8 and the new ground state appears to be an statically ordered charge and spin stripe phase [1]. It was found that this effect is connected to a structural transition from the low temperature orthorhombic phase (LTO) to the low temperature tetragonal phase (LTT). At this transition the tilt direction of the CuO_6 octahedra changes which results in different types of buckling of the CuO_2 planes. Recently several groups succeeded in preparation of LBCO thin films on various substrates which makes it possible to study the 1/8-effect under epitaxial strain [2,3]. It appears that for compressive strain (substrate: $LaSrAlO_4$) T_c increases and the 1/8-effect disappears, while in films under expansive strain [substrate: $SrTiO_3$ (STO)] T_c goes down.

Experiment and Results: The temperature dependent study of a LBCO film with x=1/8 on STO was performed at beamline X22C. The photon energy was set to 8.8 keV using a Ge(111) double-crystal monochromator. The room temperature lattice constants were determined to a_s=3.905 for STO and a_f=3.82 Å and c_f=13.266 Å for the c-axis oriented LBCO film. This has to be compared to 3.78Å and 13.28Å [1] for LBCO bulk material [1], which shows the strong expansion of the CuO_2 plane in the film. In the following film Bragg peaks will be indexed in the *Abma* notation for the LTO phase with a_f=5.4023 Å. Film super lattice reflections indicating a tilt of the CuO_6 octahedra as for example (0,3,12) or (0,3,10) were observed at any temperature up to room temperature. In contrast, no intensity was found at (h,k,l) positions connected with a LTT-type octahedra tilt pattern, as for example (1,1,8), (1,1,10), or (3,3,10). From this we have to conclude that the LBCO film – in contrast to bulk samples - exhibits a LTO-type octahedra tilt pattern for all temperatures.

At a first glance the major structural changes of the film as a function of temperature seem to be connected to the well known structural transition of STO from the cubic to the tetragonal phase (see figure). The temperature dependence of the STO reflection (0.5,0.5,2.5) shows that the transition occurs at 95 K. As for the film, however, most pronounced changes take place at about 110 K: with decreasing temperature c_f as well as a_f show a sudden drop, which means that the volume of the unit cell decreases. At the same time also the intensity of the LTO super lattice reflection (0,3,12) strongly increases signaling an increase of the octahedra tilt angle by 35%. As the intensity at the forbidden position (3,0,12) is the same, it is clear that the film is strongly twinned.

Conlcusions: Though in LBCO on STO T_c goes down, according to our results this seems not to be connected to an LTT-like buckling of the CuO_2 planes as it is the case in bulk materials. However, we find a strong increase of the LTO-like buckling which might be connected to the structural transition in STO. It would be very helpful to perform similar experiments on rare earth doped LSCO films, as the LTT phase in corresponding bulk materials is more stable than in LBCO.

Acknowledgments: The work at Brookhaven was supported by the U.S. Department of Energy, Division of Material Science, under Contract No. DE-AC02-98CH10886.

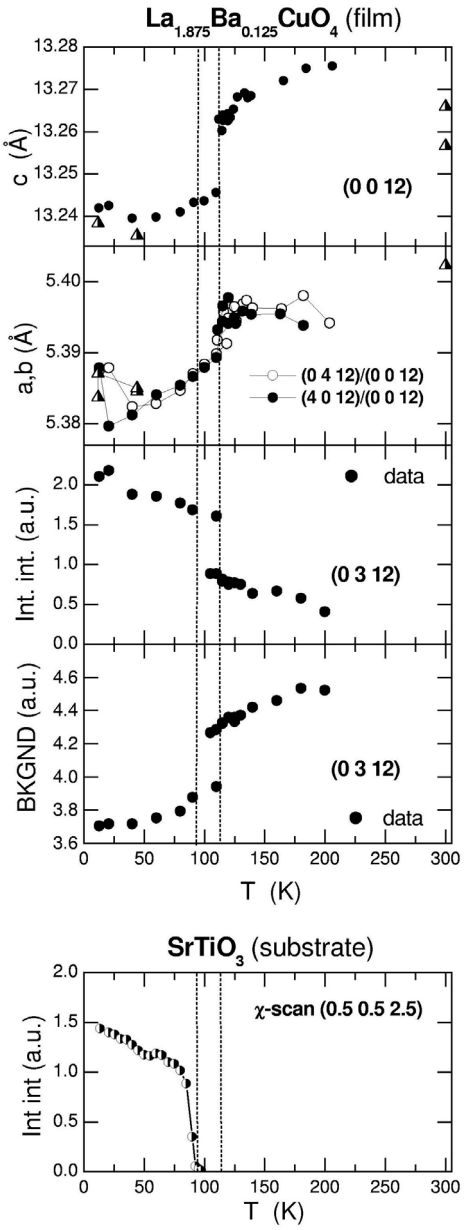

Fig.: Temperature dependence of the lattice parameters as well as integrated intensity and background signal at the (0,3,12) reflection of the LBCO film. Bottom panel: integrated intensity of the (0.5,0.5,2.5) reflection of the STO substrate.

References: [1] M. Fujita et al., Phys. Rev. B 66, 184503 (2002), [2] H. Sato et al., Phys. Rev. B 62, R799 (2000), [3] I. Tsukada et al., Phys. Rev. B 64, 224501 (2001).